

Ethyleneimine
151-56-4 | DTXSID8020599

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -79.5 °C

Global applicability domain: Inside

Local applicability domain index: 6.01e-01

Confidence level: 4.03e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyleneimine</div> <div>Measured: -77.9</div> <div>Predicted: -79.5</div>	<div>Image not found</div> <div>Allylamine</div> <div>Measured: -88.2</div> <div>Predicted: -61.3</div>	<div>Image not found</div> <div>Propyleneimine</div> <div>Measured: -65.0</div> <div>Predicted: -69.4</div>
<div>Image not found</div> <div>Isopropylamine</div> <div>Measured: -95.1</div> <div>Predicted: -39.9</div>	<div>Image not found</div> <div>Propylamine</div> <div>Measured: -83.0</div> <div>Predicted: 4.21</div>	